The operational mechanism of ferroelectric-driven organic resistive switches

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Published in:
Organic Electronics

DOI:
10.1016/j.orgel.2011.10.013

Supporting Information

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Description of the Numerical Model

The employed 2D model for ferroelectric-driven organic resistive switches takes into account the phase separated morphology, which is approximated by slabs of ferroelectric and semiconductor material that are alternating along the plane of the film in the lateral direction such that both materials are always in contact with the both the top and bottom electrode. Transport of electrons and holes is described by the drift-diffusion, continuity and Poisson equations:

$$j^n = q\mu_n nF + qD_n \nabla n \qquad \text{(S1)}$$

$$j^p = q\mu_p pF - qD_p \nabla p \qquad \text{(S2)}$$

$$q\frac{\partial n}{\partial t} = \nabla j^n + q(G-R), \qquad \text{(S3)}$$

$$q\frac{\partial p}{\partial t} = -\nabla j^p + q(G-R), \qquad \text{(S4)}$$

$$\nabla \cdot (\varepsilon \nabla \phi) = q(n-p) \qquad \text{(S5)}$$

Here ϕ denotes the electrostatic potential, F the electric field, n and p are the free carrier concentrations of electrons and holes, and j^n and j^p are the electron and hole current density, respectively. D_n, D_p, μ_n and μ_p are the diffusion coefficients and the mobilities of electrons and holes, respectively. R and G are the recombination and (photo)generation rate, respectively. The generation rate is set to zero. $\varepsilon = \varepsilon_r \varepsilon_0$ with ε_0 the permittivity of vacuum and ε_r the relative permittivity.

The recombination rate is given by the Langevin expression

$$R = \gamma np \qquad \text{(S6)}$$

with

$$\gamma = \frac{\mu_p + \mu_n}{\varepsilon} \qquad \text{(S7)}$$

The Einstein relation between diffusion constant and mobility,

$$D_{n/p} = \frac{k_B T}{q}\mu_{n/p} \qquad \text{(S8)}$$

is assumed to hold. Here, k_B is the Boltzmann constant, T the temperature, and q the elementary charge.

Eqs. (S1-S5) are solved on a rectangular 2D grid. Periodic boundary conditions on the left and right hand sides are used, effectively making the simulated device an infinite repetition of alternating slabs of ferroelectric and semiconductor material.

A Boltzmann factor for the hole and electron densities p_0, n_0 at the bottom contact is used as boundary condition for the density in the semiconductor:

$$p_0 = N_0 \exp\left(-\frac{q\varphi_p}{k_B T}\right)$$
$$n_0 = N_0 \exp\left(-\frac{q\varphi_n}{k_B T}\right) \qquad \text{(S9)}$$

The $\varphi_{p,n}$ are the effective hole and injection barriers that must add up to the HOMO-LUMO gap, *viz.* $\varphi_p + \varphi_n = E_g$. The boundary condition at the top contact is a similar Boltzmann factor. The injection barriers $\varphi_{p/n}$ may be reduced to an effective injection barrier $\varphi'_{p/n}$ by the image potential, in which case

$$\varphi'_{n/p} = \varphi_{n/p} - \sqrt{\frac{q|F|}{4\pi\varepsilon_0\varepsilon_r}} \qquad \text{(S10)}$$

The square root term in eq. (S10) only applies when the electric field F is directed to (away from) the contact so electron (hole) injection is facilitated. This model is referred to in the text as the 'Emtage O'Dwyer model' that gives rise to a field dependent charge injection.

In the ferroelectric slab a surface polarization charge density $\pm\sigma_p$ can be fixed on the first and last grid points, i.e. above the bottom electrode and below the top electrode. The sign depends on the polarization direction.

A bias V may be applied between the contacts by setting the electrostatic potential at the top contact at $-qV$ while keeping the potential of the bottom contact at zero.

Solutions to Eqs. (S1-S5) are obtained by setting the appropriate boundary conditions for n, p and φ at the start of the simulation at $t = 0$. For the rest, the device is taken to be depleted of charges at $t = 0$. In subsequent small time steps, currents are calculated from Eqs. (S1-S2), which, for each time step, give rise to a change in the carrier density according to Eqs. (S3-S4) and to a new electrostatic potential according to Eq. (S5). The changed field at the contacts translates into a change in the boundary conditions Eqs. S9 via Eq. S10. Steady state is reached when currents and carrier densities no longer change.